Transmission of Helium through Graphynes' Pores: a Quantum Mechanical Study

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Graphynes are novel two-dimensional carbon-based materials that exhibit regular and uniformly distributed sub-nanometer pores (Fig. 1). These features make them very promising materials for gas filtration applications at the molecular level[1]. Our goal is to study the interaction and dynamics of transmission of small molecules through graphynes' pores from first principles quantum mechanics calculations.

We will focus on the properties of graphdiyne (whose molecular precursor is shown in the center of FIG. 1) as a filter of ^{3}He from ^{4}He. Accurate electronic structure calculations have served to obtain a new force field suitable for molecular dynamics simulations[2]. By means of the Transition State Theory (TST)[3] we have analyzed the role of tunneling as well as of the in-pore degrees of freedom in the selectivity for isotopic separation[4]. In addition, we will present preliminary three-dimensional time-dependent wave-packet calculations of the transmission of the ^{3}He and ^{4}He through the graphynes' pores, which will allow us to compare with the results from the TST as well as with previous one-dimensional wave-packet simulations[2].

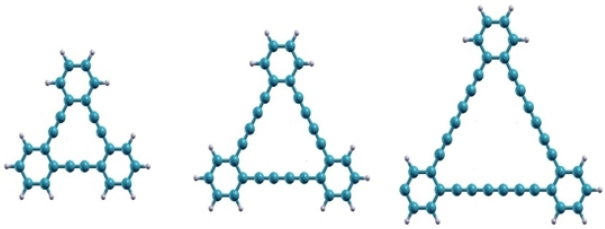

Fig. 1: Annulenic molecular precursors of graphyne, graphdiyine and graphtriyne.

References

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○ **Oral Presentation**

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